

1 1. A method for predicting a value of a property of processed material, the method
2 comprising the steps of:

3 (a) providing a process description comprising at least one governing
4 equation;

5 (b) obtaining a characterization of a flow of a material using the process
6 description;

7 (c) obtaining a morphological characterization of the material using the
8 characterization of the flow of the material; and

9 (d) predicting a value of a property of the material using the morphological
10 characterization.

1 2. The method of claim 1, wherein the process description comprises a
2 representation of an injection molding process.

1 3. The method of claim 1, wherein the process description comprises a
2 representation of at least one member of the group consisting of an extrusion process, a
3 blow molding process, a vacuum forming process, a spinning process, and a curing
4 process.

1 4. The method of claim 1, wherein the at least one governing equation comprises
2 conservation of mass, conservation of momentum, and conservation of energy equations.

1 5. The method of claim 1, wherein step (d) comprises predicting an elastic modulus
2 of the material.

- 1 6. The method of claim 5, wherein the elastic modulus is one of the group consisting
2 of a longitudinal Young's modulus, a transverse Young's modulus, an in-plane shear
3 modulus, an out-plane shear modulus, and a plane-strain bulk modulus.
- 1 7. The method of claim 1, wherein step (d) comprises predicting a complex modulus
2 of the material.
- 1 8. The method of claim 7, further comprising the step of:
2 (e) predicting a value of a property of the material from the complex modulus.
- 1 9. The method of claim 1, wherein step (d) comprises predicting at least one member
2 of the group consisting of a mechanical property, a thermal property, and an optical
3 property.
- 1 10. The method of claim 1, wherein step (d) comprises predicting at least one of a
2 thermal expansion coefficient, a thermal conductivity, a bulk modulus, and a sound
3 speed.
- 1 11. The method of claim 1, wherein step (d) comprises predicting at least one of
2 clarity, opaqueness, surface gloss, color variation, birefringence, and refractive index.
- 1 12. The method of claim 1, wherein step (d) comprises predicting at least one
2 component of a stress tensor.
- 1 13. The method of claim 12, wherein the stress tensor comprises a measure of flow-
2 induced stress.
- 1 14. The method of claim 1, wherein the morphological characterization comprises at
2 least one component of a conformation tensor.
- 1 15. The method of claim 1, wherein the morphological characterization comprises at
2 least one component of an orientation tensor.

- 1 16. The method of claim 1, wherein the morphological characterization comprises a
2 measure of crystallinity.
- 1 17. The method of claim 16, wherein the measure of crystallinity is a measure of
2 relative crystallinity.
- 1 18. The method of claim 1, wherein step (c) comprises obtaining the morphological
2 characterization using a description of crystallization kinetics of the material.
- 1 19. The method of claim 18, wherein the description of crystallization kinetics of the
2 material comprises a dimensionality exponent.
- 1 20. The method of claim 18, wherein the description of crystallization kinetics of the
2 material comprises a description of flow-induced free energy change.
- 1 21. The method of claim 18, wherein the description of crystallization kinetics of the
2 material comprises a description of flow-induced nucleation.
- 1 22. The method of claim 1, wherein step (c) comprises obtaining the morphological
2 characterization using a two-phase description of the material.
- 1 23. The method of claim 22, wherein the two-phase description comprises at least one
2 of a crystallization kinetics model, an amorphous phase model, and a semi-crystalline
3 phase model.
- 1 24. The method of claim 22, wherein the two-phase description comprises a
2 crystallization kinetics model, an amorphous phase model, and a semi-crystalline phase
3 model.
- 1 25. The method of claim 22, wherein the two-phase description comprises a
2 viscoelastic constitutive equation that describes an amorphous phase.

- 1 26. The method of claim 25, wherein the viscoelastic constitutive equation comprises
2 a FENE-P dumbbell model.
- 1 27. The method of claim 25, wherein the viscoelastic constitutive equation comprises
2 at least one of an extended POM-POM model and a POM-POM model.
- 1 28. The method of claim 25, wherein the viscoelastic constitutive equation comprises
2 at least one of a Giesekus model and a Phan-Thien Tanner model.
- 1 29. The method of claim 22, wherein the two-phase constitutive description
2 comprises a rigid dumbbell model that describes a semi-crystalline phase.
- 1 30. The method of claim 1, further comprising the step of:
2 (e) performing a structural analysis of a product made from the processed
3 material using the value of the property of the material.
- 1 31. The method of claim 30, wherein step (e) comprises predicting warpage of the
2 product.
- 1 32. The method of claim 30, wherein step (e) comprises predicting shrinkage of the
2 product.
- 1 33. The method of claim 30, wherein step (e) comprises predicting how the product
2 reacts to a force.
- 1 34. The method of claim 30, wherein step (e) comprises predicting at least one of the
2 group consisting of crack propagation, creep, and wear.
- 1 35. The method of claim 30, wherein step (e) comprises predicting at least one
2 member of the group consisting of impact strength, mode of failure, mode of ductile
3 failure, mode of brittle failure, failure stress, failure strain, failure modulus, failure

4 flexural modulus, failure tensile modulus, stiffness, maximum loading, and burst
5 strength.

1 36. The method of claim 1, wherein obtaining the flow characterization comprises
2 using a dual domain solution method.

1 37. The method of claim 1, wherein obtaining the flow characterization comprises
2 using a hybrid solution method.

1 38. The method of claim 1, wherein step (b) is performed after each of a plurality of
2 time steps associated with a solution of the at least one governing equation in step (a).

1 39. The method of claim 1, wherein steps (b) and (c) are performed after each of a
2 plurality of time steps associated with a solution of the at least one governing equation in
3 step (a).

1 40. The method of claim 1, wherein steps (b), (c), and (d) are performed after each of
2 a plurality of time steps associated with a solution of the at least one governing equation
3 in step (a).

1 41. The method of claim 1, wherein step (c) comprises performing one or more
2 crystallization experiments to determine one or more parameters used to obtain the
3 morphological characterization.

1 42. The method of claim 1, wherein step (c) comprises performing one or more
2 crystallization experiments to determine a crystal growth rate of the material under
3 quiescent conditions.

1 43. The method of claim 1, wherein step (c) comprises performing one or more
2 crystallization experiments to determine a half-crystallization time.

1 44. The method of claim 1, wherein step (c) comprises performing one or more
2 experiments to determine at least one of a relaxation spectrum and a time-temperature
3 shift factor.

1 45. A method for performing a structural analysis of a manufactured part, the method
2 comprising the steps of:

3 (a) providing a process description comprising at least one governing
4 equation;

5 (b) obtaining a characterization of a flow of a material using the process
6 description;

7 (c) obtaining a morphological characterization of the material using the
8 characterization of the flow of the material;

9 (d) predicting a value of a property of the material using the morphological
10 characterization; and

11 (e) performing a structural analysis of a part made from the material using the
12 predicted value of the property.

1 46. The method of claim 45, wherein step (e) comprises creating a structural analysis
2 constitutive model.

1 47. The method of claim 45, wherein step (e) comprises predicting a response of the
2 part to a load.

1 48. The method of claim 45, wherein step (e) comprises predicting warpage of the
2 part.

1 49. The method of claim 45, wherein step (e) comprises predicting at least one
2 member of the group consisting of warpage, shrinkage, crack propagation, creep, wear,
3 lifetime, and failure.

1 50. A method for designing a part, the method comprising the steps of:

2 (a) providing a test design of a part, wherein the part is made from a material;

3 (b) providing a process description comprising at least one governing
4 equation applied within a volume, wherein the volume is based on the test design of the
5 part;

6 (c) obtaining a characterization of a flow of the material using the process
7 description;

8 (d) obtaining a morphological characterization of the material using the
9 characterization of the flow of the material;

10 (e) predicting a value of a property of the material using the morphological
11 characterization;

12 (f) using the value of the property to evaluate a measure of part performance;
13 and

14 (g) determining whether the measure of part performance satisfies a
15 predetermined criterion.

1 51. The method of claim 50, wherein the method further comprises the step of:

2 (h) modifying the test design in the event that the measure of part
3 performance does not satisfy the predetermined criterion.

1 52. A method for designing a manufacturing process, the method comprising the steps
2 of:

- 3 (a) providing a test set of inputs for a process for manufacturing a product
4 from a material;
- 5 (b) providing a description of the process, the description comprising at least
6 one governing equation;
- 7 (c) obtaining a characterization of a flow of the material using the description
8 of the process and the test set of inputs;
- 9 (d) obtaining a morphological characterization of the material using the
10 characterization of the flow of the material;
- 11 (e) predicting a value of a property of the material using the morphological
12 characterization;
- 13 (f) using the value of the property to evaluate a measure of product
14 performance; and
- 15 (g) determining whether the measure of product performance satisfies a
16 predetermined criterion.

1 53. An apparatus for predicting a value of a property of processed material, the
2 apparatus comprising:

- 3 (a) a memory that stores code defining a set of instructions; and
- 4 (b) a processor that executes the instructions thereby to:
- 5 (i) obtain a characterization of flow of a material using a process
6 description comprising at least one governing equation;
- 7 (ii) obtain a morphological characterization of the material using the
8 characterization of flow of the material; and

9 (iii) predict a value of a property of the material using the
10 morphological characterization.

1 54. A method for predicting a value of a property of processed material, the method
2 comprising the steps of:

3 (a) providing a process description comprising at least one governing
4 equation;

5 (b) obtaining a characterization of a flow of a material using the process
6 description;

7 (c) providing a two-phase description of the material, wherein the description
8 is based in part on the characterization of the flow of the material;

9 (d) obtaining a morphological characterization of the material using the two-
10 phase description; and

11 (e) predicting a value of a property of the material using the morphological
12 characterization.

1 55. The method of claim 54, wherein the material undergoes a change of phase during
2 processing.

1 56. The method of claim 54, wherein the two-phase description comprises an
2 amorphous phase model and a semi-crystalline phase model.

1 57. A method for simulating fluid flow within a mold cavity, the method comprising
2 the steps of:

3 (a) providing a representation of a mold cavity into which a material flows;

4 (b) defining a solution domain based on the representation; and

5 (c) solving for a process variable in the solution domain at a time t using at
6 least one governing equation, wherein step (c) comprises the substep of using a
7 morphological characterization of the material in solving the at least one governing
8 equation.

1 58. The method of claim 57, wherein the substep of using a morphological
2 characterization of the material in solving the at least one governing equation comprises
3 determining a viscosity of the material based at least in part on the morphological
4 characterization of the material.

1 59. The method of claim 57, wherein the substep of using a morphological
2 characterization of the material in solving the at least one governing equation comprises
3 determining a viscosity of the material based at least in part on the morphological
4 characterization of the material at a time prior to the time t .

1 60. A method for predicting a morphological characteristic of structures within a
2 manufactured part, the method comprising the steps of:

- 3 (a) providing a model of at least one stage of a manufacturing process;
4 (b) obtaining a characterization of flow of a material, where the flow occurs
5 during the at least one stage of the manufacturing process; and
6 (c) predicting a morphological characterization of structures within at least a
7 portion of a manufactured part using the flow characterization.

1 61. The method of claim 60, wherein step (c) comprises predicting an orientation of
2 crystallites within the manufactured part.

1 62. The method of claim 60, wherein step (c) comprises predicting a size distribution
2 of crystallites within the manufactured part.

- 1 63. The method of claim 60, wherein step (c) comprises predicting a crystal volume
2 as a function of position within the manufactured part.
- 1 64. The method of claim 60, wherein step (c) comprises predicting an orientation
2 factor as a function of position within the manufactured part.
- 1 65. The method of claim 60, wherein step (c) comprises predicting the morphological
2 characterization using a description of crystallization kinetics of the material.
- 1 66. The method of claim 65, wherein the description of crystallization kinetics
2 comprises an expression for excess free energy.
- 1 67. The method of claim 60, wherein the manufacturing process is an injection
2 molding process.
- 1 68. The method of claim 1, wherein step (d) comprises predicting material property
2 values at a plurality of locations within a part made from the processed material.
- 1 69. The method of claim 1, wherein step (d) comprises predicting material property
2 values of a part having an arbitrary geometry, where the part is made from the processed
3 material.
- 1 70. The method of claim 3, wherein the process description comprises a
2 representation of at least one member of the group consisting of a profile extrusion
3 process, a blow film extrusion process, and a film extrusion process.
- 1 71. The method of claim 45, wherein step (e) comprises predicting a response of the
2 part to a thermal load.